

PFOA

335-67-1 | DTXSID8031865

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: -12.1 cm³/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 2.50e-01

Confidence level: 5.80e-01

Nearest Neighbors from the Training Set

[Image not found](#)

1,1,2,3,3,3-Hexafluoro-1-propene

Measured: -11.7

Predicted: -11.7

[Image not found](#)

Acetic acid, trifluoro-

Measured: -12.9

Predicted: -12.7

[Image not found](#)

Trifluoro(trifluoromethoxy)ethylene

Measured: -11.4

Predicted: -11.5

[Image not found](#)

Acetic acid, trifluoro-, methyl ester

Measured: -13.3

Predicted: -13.3

[Image not found](#)

Chlorotrifluoroethylene

Measured: -11.2

Predicted: -11.2